# Robust approximation of the conditional mean for applications of Machine Learning

Amy Parkes<sup>a,\*</sup>, Josef Camilleri<sup>b</sup>, Dominic Hudson<sup>a</sup>, Adam Sobey<sup>a,c</sup>

#### 4 Abstract

Machine Learning approaches are increasingly used in a range of applications. They are shown to produce low conventional errors but in many real applications fail to model the underlying input-output relationships. This is because the error measures used only predict the conditional mean under some restrictive assumptions, often not met by the data we extract from applications. However, new approaches to Machine Learning, for example using Evolutionary Computation, allow a range of alternative error measures to be used. This paper explores the use of the Fit to Median Error measure in machine learning regression automation, using evolutionary computation in order to improve the approximation of the ground truth. When used alongside conventional error measures it improves the robustness of the learnt input-output relationships to the conditional median. It is compared to traditional regularisers to illustrate that the use of the Fit to Median Error produces regression neural networks which model more consistent input-output relationships. The problem considered is ship power prediction using a fuel-saving air lubrication system, which is highly stochastic in nature. The networks optimised for their Fit to Median Error are shown to approximate the ground truth more consistently, without sacrificing conventional Minkowski-r error values.

- 5 Keywords: Machine Learning, Genetic Algorithms, Neural Architecture
- 6 Search, Optimisation, Application

 <sup>&</sup>lt;sup>a</sup> Maritime Engineering, University of Southampton, Southampton, SO17 1BJ, UK
 <sup>b</sup> Silverstream Technologies Ltd, 1 St Vincent Street, London, W1U 4DA, UK
 <sup>c</sup> Data-centric Engineering, The Alan Turing Institute, The British Library, NW1
 2DB, London, UK

## 1. Robust approximation of the ground truth

Machine learning regression models are increasingly being used in industrial and engineering contexts for high-stakes decision making, automation and control. These methods often produce low conventional error values, yet only 10 produce physically inconsistent results under a number of assumptions [3], which are often not met in real applications. Outside of these contraints they cannot generalise off test set and so cannot be relied upon to model the ground truth 13 of the system. In real-world applications, where the output can have a direct effect on human life or the environment, model accuracy alone is not sufficient. It 15 has been demonstrated that for many applications minimising traditional error measures cannot guarantee an accurate approximation of the ground truth [28]. This is due to a poor inductive bias, the inherent prioritisation of one solution 18 over another [2], produced by conventional error measures which are based on Minkowski-r metrics [10]. 20 This trust can be increased by manually tuning to remove overfitting or to 2: provide a solution that makes more sense to the user. However, the expert knowledge and domain experience required to properly tune a machine learn-23 ing method manually are not always available in industry. Genetic algorithms are also increasingly used to search a method's hyperparameter space more efficiently [29] [15] [1]; which minimise conventional error measures on a test set, often combined with lowering the complexity of the network. This automation 27 exacerbates the lack of interpretability, as models have a large flexibility, and 28 prediction accuracy is prioritised. A low conventional error is often achieved without certainty that the method has modelled the correct internal functions. Regularisation hyperparameters can be optimised alongside other neural network parameters [26] [19], which increases the search space and creates more flexibility for methods to produce 'accurate' predictions and avoid overfitting. 33 These approaches improve the modelling of the ground truth in scenarios adhering to the assumptions in the proof in [3], which are

# 1. the datapoints are independent;

- 2. the distribution of the target variable is to be deterministic of the input with Gaussian noise, e.g.  $y = \phi(x) + \epsilon$  where  $\phi$  depends only on input variable x, and  $\epsilon \sim N(0, \sigma^2)$ ;
- 3. the standard deviation of noise,  $\sigma$ , is not dependent on the input x;
- 4. and the data set and neural network must be sufficiently large.

and under which minimum Minkowski-r error values approximate the condi-42 tional average of the dataset. This is because the inductive bias from the loss 43 function guides the input-output relationships towards the conditional average, while the regularisation stops overfitting by simplfying the input-output relationships being modelled. However, these assumptions are restrictive and it is noted that few regression applications adhere to them. For example, one assumption is that the dataset is homoscedastic. In scenarios not adhering to these 48 assumptions, network regularisation simplifies the relationships being modelled but this does not necessarily improve the generality, or model the ground truth. The Fit to Median Error measure [22] produces models with a better fit to 51 the true input-output relationships, when used in conjunction with conventional 52 error measures. The use of this error measure removes the need for assumptions 53 2. and 3. to hold to model the ground truth. Which is achieved by regularising the learnt input-output relationships to the conditional median of the training dataset: the median output value, conditioned on each isolated input variable 56 in turn [3]. For many regression applications the conditional medians are a good 57 approximation of the ground truth input-output relationships, and therefore bi-58 asing the input-output relations learnt by the regression method towards the conditional medians produces models with more robust input-output relationships. The Fit to Median Error measure has been shown to produce models 61 with a better approximation of the true input-output relations by trialling it on 62 an artificial dataset, where the input-output relations can be fully defined, the 63 results of this study can be found in [22]. As yet, the Fit to Median error it has not been explored as part of an automated approach.

This paper therefore explores the automation of neural network training to a

new problem, with a focus on producing a network which accurately models the ground truth. To achieve this, the cMLSGA multi-objective genetic algorithm is used to tune the hyperparameters of neural networks. The study compares the ground truth representation of a neural network when a genetic algorithm optimises the network's hyperparameters to reduce the Mean Fit to Median Error measure and compares it to standard regularization using 11, 12 and dropout, and to a network optimised to minimise the Maximum Absolute Error. It is illustrated that neural network regularisation methods (11, 12 and dropout) can be replaced by the use of the Mean Fit to Median performance measure as an objective in the genetic algorithm, reducing the complexity of the search space and producing networks which more consistently model the ground truth.

## 2. Neural Networks Parameters

A challenging regression problem is ship power prediction for a vessel using 79 air lubrication to reduce fuel consumption. It is chosen to be used in this study 80 as it violates the assumptions in [3], where the noise in the output space is non-81 Gaussian and heteroscedastic, it is also likely that there is not enough data. In this situation, correctly modelling the ground truth and accurate prediction is required but there is limited understanding of the ground truth [21], meaning 84 physics-informed approaches are not applicable. The literature shows that shaft powering of a vessel can be predicted with average accuracies of between 1.5-5% 86 error with the use of a regression neural network trained with high frequency data from the vessel [23], [24], [16], [12] and [18]. All neural network applications to ship power prediction in the literature use a combination of local searches and domain knowledge to identify hyperparameter values. The addition of an air lubrication device increases the complexity of the regression problem, as the 91 system interacts with a number of interrelated input variables.

Previous applications of neural networks to ship power prediction use between 1 and 3 hidden layers [17] [20], and between 5 and 300 neurons in each hidden layer [12]. To provide a sufficiently large search space to allow verification, or otherwise, of these parameters a maximum of 4 hidden layers and 1000 neurons in each layer are used. The majority of the literature treats the problem as time-invariant and use feed-forward networks, so no recurrent parameters are optimised. As the optimiser or activation functions are rarely documented in the literature, the state-of-the-art optimisers and activation functions available in the Keras framework [4] are used in the optimisation, Table 1.

Table 1: Selected Neural Network Hyperparameters

Hyperparameter	Value or set
Layers	[1,4]
Neurons in each	[1,1000]
layer	
Epochs	Increasing from 1-20 for increasing generations
Early stopping pa-	5
tience	
Loss function	Mean Absolute Error
Performance mea-	Mean Absolute Relative Error, Maximum Absolute
sures	Relative Error, Mean Fit to Median Error
Optimiser	SGD, Adam [14], Nadam [5],
	RMSprop [11], Adagrad [6],
	Adadelta [30], Adamax [14]
Activation function	ReLU, sigmoid, softmax, softplus, softsign, tanh,
	selu, elu
11 & 12 Rates	0, 0.01,0.001,0.0001,0.00001
Dropout	[0,0.9)
Initialiser	Random Normal ( $\mu = 0, \sigma = 0.1$ )

The number of epochs and early stopping procedure are not optimised, as 102 there was a need for predictable compute requirements and allowing the opti-103 misation of these parameters leads to unpredictable run times. The number of 104 epochs to train each network increases for increasing generation number in the 105 genetic algorithm, from 1 epoch in the first 15 generations to 20 in the final 15. 106 This was also implemented to reduce compute and it was validated that when 107 more than 20 epochs were allowed, that the early stopping, with a patience of 108 5, stopped the training within 20 epochs for the majority of networks. The loss 109 function is similarly not optimised, the Mean Absolute Error is used, as the 110 conditional medians are closer to the ground truth input-output relationships 111 in these datasets than the conditional means. 112

The performance measures, or the genetic algorithm's fitness functions, are 113 the Mean Absolute Relative Error, the Maximum Absolute Relative Error and 114 the Mean Fit to Median Error. Different combinations of these, alongside the use of L1, L2<sup>1</sup> and dropout<sup>2</sup> regularisation parameters in the search space are 116 compared to illustrate the effect of different types of regularisation. 117

#### 3. cMLSGA Parameters 118

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Table 2: Selected cMLSGA Hyperparameters

Hyperparameter	Value or set
Algorithm at Individual Level	HEIA, IBEA
Crossover Type & Rate	SBX & DE, 1
Mutation Type & Rate	Polynomial,
	0.08
Number of eliminated collectives	1
Generations between elimination	10
Population size	1000
Generations	300
Proportion elite	10%

In this study cMLSGA<sup>3</sup> is selected as it shows the top performance on a 119 range of evolutionary benchmarking problems [9] and practical problems [8]. 120 Genetic algorithms are increasing used to tune neural network hyperparame-121 ters including regularisation parameters for use on new problems [13]. Many 122 approaches have multiple genetic algorithm objectives, although these all min-123 imise an error measure and a measure of network complexity [27] and [25]. The 124 use of multiple different performance measures as objectives is yet to be explored 125 126 in the literature.

Four approaches are investigated in this study, summarised in Table 3, for approach (GAi) and (GAii) the genetic algorithm cMLSGA optimises all vari-

<sup>&</sup>lt;sup>1</sup>L1 and L2 encourage simple relationships to be modelled by penalising large weights. L1 adds the absolute values of the weights to the cost function and L2 adds the squared values of the weights to the cost function.

<sup>&</sup>lt;sup>2</sup>Dropout works by turning off a certain proportion of neurons randomly at each run of the network, and it's use is shown to be equivalent to using a Bayesian network [7] 

The code for cMLSGA is available at https://github.com/12yuens2/cmlsga-jmetalpy.

Table 3: Genetic Algorithm Approaches

Approach	Objective(s)	Network Regularisation
		Tarisation
GAi	Mean Absolute Error	l1, l2 and
		dropout
GAii	Mean Absolute Error	11, 12 and
		dropout
	Maximum Absolute Error	
GAiii	Mean Fit to Median Error	None
	Mean Absolute Error	
GAiv	Mean Absolute Error	None
	Maximum Absolute Error	

ables in Table 2, including the l1 and l2 regularisation rate and the dropout rate of the networks. Although it is advised that l2 regularisation and dropout are not used in the same network the genetic algorithms are provided with zero options for all regularisation parameters, to identify if one is preferable in this scenario.

Approach (GAi) is a single objective genetic algorithm optimising the Mean 134 Absolute Error which is compared to a multi-objective formulation where the 135 (GAii) approach optimises both Mean Absolute Error and Maximum Absolute 136 Error. For approaches (GAiii) and (GAiv) no network regularisation parame-137 ters are optimised: 11, 12 and dropout rates are all set permanently to zero. They 138 avoid producing networks that have overfitted by the use of two performance 139 metrics as multi-objectives, (GAiii) uses the Mean Fit to Median and Mean 140 Absolute Errors to be minimised and (GAiv) uses the Maximum Absolute and Mean Absolute. All approaches use 40 CPUs with 2.0 GHz Intel Skylake processors and 192 GB of DDR4 memory, and take less than 3 days, this setup may 143 not be feasible for widespread industrial application, although it is suggested it 144 is within reach of some industries. 145

#### 146 4. Data

The data used in this study are from a large vessel equipped with the Silverstream®Air Lubrication System. The air lubrication system works through use

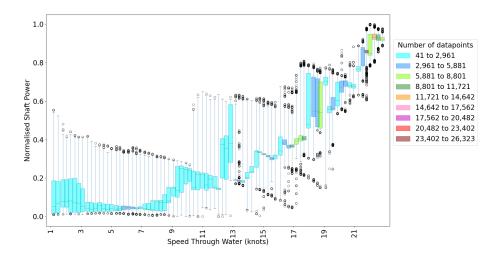


Figure 1: The distribution of the observed shaft powers for half knot bins of speed through the water for dataset where the system is off. In the box and whisker plots the boxes contain 50% of the distribution and the whiskers extend to the datum which is at 1.5 times the interquartile range.

of fluid sheering to create an air microbubble carpet directly captured within the boundary layer on the ship hull bottom. The bubble carpet reduces the frictional resistance thereby increasing the speed and reducing the shaft power. Compressors provide a constant supply of air to the hull bottom to maintain a uniform bubble carpet operated at the optimal compressor power that maximises the energy balance. The study is performed on both system on and system off datasets, however for brevity only results for system off are presented as they show similar performance. This prediction is required for a baseline determination of how the system is working, but the relationships between the power, weather, ocean and operating conditions are complex and difficult to model.

The variables considered in this study are the shaft power, speed through water, relative wind speed and direction, draught and trim, with shaft power the target variable. These are selected based on a detailed study into variable selection for shaft power prediction [20]. The speed through water is selected over the speed over ground, for use as an input variable, as it is more hydrody-

manically relevant and its accuracy is validated by comparison to the speed over 165 ground. The dataset is cleaned by removing rows with missing or non-physical 166 values and all datapoints below 0.05 normalised shaft power are removed. The dataset is split into two using the air lubrication system status: system on and 168 system off, where system on is defined as air lubrication system power greater 169 than zero. The system on dataset contains 352,690 datapoints and system off 170 contains 237,962. The data is split into training, testing and validation sets of 171 70%, 15% and 15% respectively. Each network in the genetic algorithm trains 172 on a randomly sampled 35,000 datapoints from the training set and uses ran-173 domly sampled sets of size 7,500 from validation and testing sets for validation 174 during training, and testing to produce the fitness of the network for the ge-175 netic algorithm. The errors stated in the paper are from networks on the Pareto 176 fronts of each approach, which are validated on the full testing set.

The datasets contain large regions of sparse data in all input variable do-178 mains, this is exemplified by the ship speed domain where each half-knot interval 179 below 16 knots contains less than 0.8% of the data, which accounts for more than 180 half the speed domain, Figure 1. In addition, the boxplot ranges and outliers 181 show high heteroscedicity with idiosyncratic noise caused by situations where 182 the angle of the propeller blades is varied to achieve the required speed. This 183 highlights the complexity in developing models of the powering of this vessel, as 184 the dataset also contains the effects from other latent variables, such as piloting 185 behaviour and route taken.

## 5. Optimisation including regularisation parameters: (GAi) and (GAii)

Previous studies predicting ship powering using neural networks report that 11, 12 and elastic net increase both test set and off-test set errors and that optimal values for both 11 and 12 are zero. Therefore the genetic algorithm setup is biased towards low and zero values of regularisation rates by using a set of exponentially decreasing values and an explicit zero option.

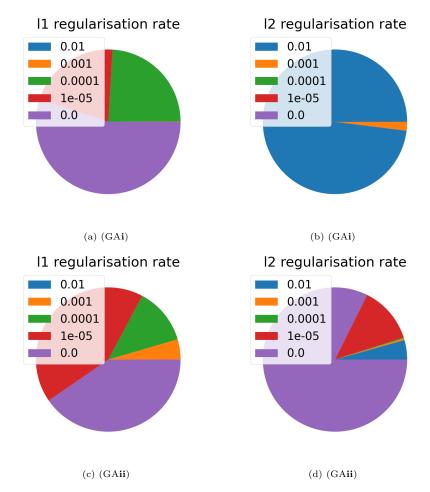
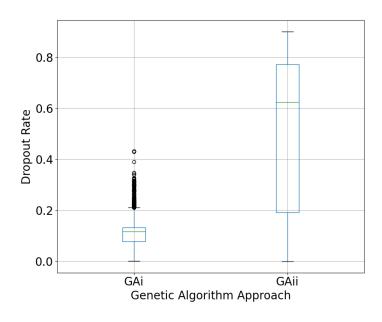


Figure 2: Distribution of regularisation rates for networks in the last 15 generations of (GAi) cMLSGA with multi-objectives of minimising Maximum and Mean Absolute Error for (a) 11 and (b) 12 and (GAii) cMLSGA with the single objective of minimising Mean Absolute Error for (c) 11 and (d) 12

The single objective (GAi) fails to identify that zero regularisation rates produce the lowest errors, favouring networks with the highest possible rate of 12 (0.01), Figure 2b. (GAi) produces networks with the highest Mean Absolute Relative Errors of all the approaches,  $(5.19\pm0.00)\%$  from Figure 4a. In contrast, (GAii) favours lower 11 and 12 rates of 0 or 0.00001, Figures 2c and 2d, which results in networks with the lowest Mean Absolute Relative Errors of all four approaches, on average, with a value of  $(2.87\pm0.45)\%$ , shown in Figure 4a.



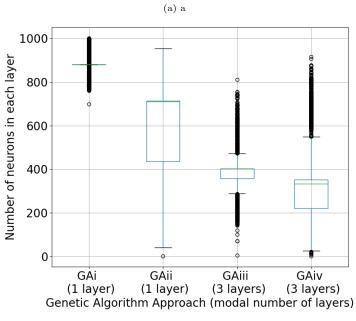


Figure 3: (a) Dropout rate for networks in the last 15 generations of cMLSGA with (GAi) the single objective of minimising Mean Absolute Error and (GAii) multi-objectives of minimising Maximum and Mean Absolute Error and (b) the number of neurons in each layer for networks in the last 15 generations of cMLSGA with (GAi), (GAii), (GAiii) and (GAiv).

(b) b

This is around 0.5% higher than the lowest documented error for ship power prediction.

It is posited that the high error for the single objective problem is directly related to the use of a large 12 regularisation rate, as noted in previous studies 203 for ship power prediction. It is possible that the use of a multi-objective search 204 algorithm for a single-objective problem means that the optimal hyperparame-205 ters can't be found, resulting in large errors. The implementation also requires restrictions in the number of epochs used for training in the initial generations, it is possible this biases (GAi) towards certain size networks, where higher l2 208 rates are preferable. This hypothesis is supported by the fact that 74.4% of 209 networks in the first 15 generations of (GAi) have 1 hidden layer, and that 210 over 99.8% of the networks in the final 15 generations have 1 hidden layer, with 211  $880\pm17$  neurons in this layer, Figure 3b. This is significantly more neurons than those in the hidden layer of networks in the final 15 generations of (GAii) which 213 range from 3-952 with a median value of 709, Figure 3b. The added objective of 214 minimising Maximum Absolute Error in (GAii) may cause these slightly smaller 215 networks to be more attractive as they are in a sense regularised by their size, 216 as they have reduced modelling flexibility therefore are less likely to overfit and 217 produce high Maximum Absolute Errors. 218

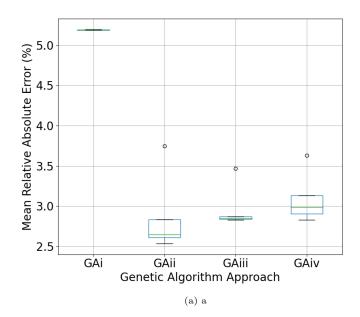
Another explanation for the difference in 12 rates chosen by (GAi) and (GAii) 219 is the equivalence of 12 and dropout. Since 12 and dropout are equivalent up 220 to a Fisher transformation, their use in conjunction is not recommended. The evidence for this is that (GAi) favours the highest 12 rate and has a median 222 dropout rate in the final 15 generations of 0.116, whereas (GAii) favours the 223 zero 12 rate and has a median dropout rate of 0.624, Figure 3a. This illustrates 224 that the genetic algorithms will chose either 12 or dropout to minimise the Mean 225 Absolute Relative Error. The 11 rates also support this hypothesis, as chosen 226 rates for l1 regularisation in the final 15 generations are more comparable for (GAi) and (GAii). 228

# 6. Optimisation using multiple performance measures: (GAiii) and (GAiv)

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For approaches (GAiii) and (GAiv) all neural network regularisation param-231 eters are set to zero. The regularisation is performed by minimising different network performance measures, the Mean Absolute and Mean Fit to Median for 233 (GAiii), and the Mean Absolute and Maximum Absolute for (GAiv). The trade-234 off between the two objectives produces regularised neural networks, without 235 explicitly changing the architecture or loss function. The Mean Fit to Median is chosen as it indicates how close the relationships modelled by a network are to 237 the conditional averages of the dataset, in many regression examples this is akin 238 to the ground truth input-output relationships [22]. The Maximum Absolute 239 is chosen as for many industrial applications of machine learning the maximum 240 prediction error is more pertinent than the mean error. The Mean Absolute Error is used instead of the Mean Squared Error in both approaches, as the conditional medians are closer to the ground truth input-output relationships 243 in these datasets than the conditional means. 244

Differently shaped networks are favoured by (GAiii) and (GAiv), compared to (GAi) and (GAii), focusing on networks with 3 hidden layers and on average less than 400 neurons in each layer, Figure 3b. These networks have 51 times 247 the number of connections than the networks chosen in (GAi) and (GAii). 248 Apart from (GAi), (GAiii) has the most consistently sized networks in the 249 final 15 generations, with an interquartile range of 46 neurons, compared to 250 (GAiv) which have an interquartile range of 131 neurons. It is suggested that as the Mean Fit to Median Error biases networks towards specific input-output 252 relationships, there is a smaller range of potential network architectures which 253 habitually model these relationships. Whereas networks which minimise the 254 Maximum Absolute Error are less restricted and can model a wider range of 255 input and output relationships.



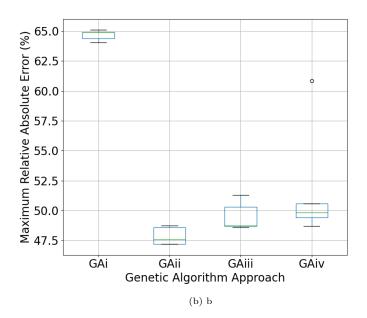


Figure 4: (a) Mean Relative Absolute Error and (b) Maximum Absolute Error from cMLSGA with (GAi) the single objective of minimising Mean Absolute Error and (GAii) multi-objectives of minimising Maximum and Mean Absolute Error, both optimising the parameters for 11, 12 regularisation and dropout in the networks, and (GAiii) and (GAiv) which do not use network regularisation but minimise Mean Fit to Median and Maximum Absolute Error respectively, alongside Mean Absolute Error

The Mean Absolute Relative Errors from networks in the Pareto fronts 257 are  $(2.97 \pm 0.25)\%$  for (GAiii) and  $(3.10 \pm 0.28)\%$  for (GAiv). It is expected 258 that (GAiv) would produce higher Mean Absolute Relative Errors as discussed above, minimising the Maximum Absolute Error should bias predictions to-260 wards the midpoint of the conditional output distributions, whereas minimising 261 the Mean Absolute Error should bias predictions towards the median of these 262 distributions. As it is established that noise in the output distribution is non-263 Gaussian, Figure 1, these values will not align so some sacrifice in Mean Absolute Error is expected from (GAiv). Both (GAiii) and (GAiv) produce comparable 265 Maximum Absolute Errors, of  $(49.5 \pm 1.1)\%$  and  $(51.9 \pm 4.5)\%$ . It is suggested 266 that this is because, although the conditional median output value and condi-267 tional midpoint output value do not align for the majority of the input domain, they are sufficiently close to produce comparable Maximum Absolute Errors. Across all four approaches, the genetic algorithm producing networks with 270 the highest Mean Absolute Error is the approach which does not provide extra 271 weighting to sparse areas of data. The approaches minimising Maximum Absolute Error are implicitly biased away from networks which predict the majority of the testing datapoints correctly, but predict one datapoint poorly, favouring networks which predict all testing datapoints to a moderate degree of error. Approach (GAiii) more explicitly weights prediction in sparse areas of data by

272 273 274 275 276 favouring networks which model the conditional median of the dataset across all 277 input domains, irrespective of the quantity of data across each input domain. The regression problem of ship power prediction is chosen in part because of it's 279 irregular data distribution; more than 9% of the dataset lies in less than a 0.5 280 knot interval of ship speed, Figure 1. This provides an explanation for the high 281 testing errors from (GAi), where only the Mean Absolute Error is minimised, 282 there is little incentive for the genetic algorithm to produce networks which 283 generalise across the full range of the input domain well.

## 7. Comparison of the ground truth approximation

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Five networks selected from the four different approaches the learnt relationship between an input, the ship speed, and the output, shaft power, for the networks in the Pareto front of each approach are visualised, Figure 5. These are extracted with the following procedure: set all but one input variable to be constant at the mode; cycle the remaining variable from its minimum to its maximum recorded values with 150 points evenly spaced along the domain and run the new dataset through the trained network.

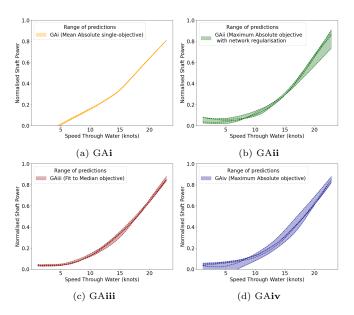


Figure 5: The learnt speed-power curves from 5 networks on the Pareto fronts of (GAii), (GAiii), (GAiv) and the 5 networks producing lowest Mean Absolute Relative Error from (GAi).

The approach which produces the most consistent speed-power relationships is (GAi), with an average variation of 1.8%<sup>4</sup>, Figure 5a. However, the relationships ship modelled by the 5 networks with the lowest Mean Absolute Relative Error

 $<sup>^4</sup>$  Average variation in just the speed-power curves are discussed in this section, but it is verified that all input-power curves follow the same trends with variation around 0.5% across input variables.

in (GAi) all approximate a piece-wise linear relationship which clearly underfits the dataset in Figure 1. The expected trend between ship speed through the 297 water and shaft power is a cubic polynomial, therefore as well as producing the highest Mean Absolute Relative Errors, networks chosen by (GAi) model the 299 ground truth input-output relationships the worst out of the four approaches. 300 Both (GAii) and (GAiv) produce 5 fairly consistent speed-power curves, with 301 average variations of 5.9% and 10% respectively, Figures 5b and 5d. Both ap-302 proaches approximate smooth polynomial curves, although the degrees of the polynomials might differ, as multiple curves intersect at various points along 304 the speed axis. The spread of learnt relationships is greater at the highest and 305 lowest speeds for (GAii), with a decrease in spread for speeds of around 15 306 knots, where many of the curves intersect. The curves from (GAiv) show equal spread across the speed domain.

The approach with both accurate and consistent learnt speed-power curves 309 is (GAiii), with limited intersections of curves and an average spread of 3.0%. 310 It is suggested that the reason using the Mean Fit to Median Error as an ob-311 jective in a multi-objective genetic algorithm produces more consistent learnt 312 relationships, is because instead of encouraging the networks to model more 313 simple relationships it encourages the networks to model the conditional me-314 dian functions of the dataset, supported by the increase in network connections. 315 Whereas the other approaches leave room for networks to fail to model the 316 conditional averages, especially in irregularly distributed and non-normally distributed datasets. The Mean Absolute Error values from networks selected by 318 (GAiii) are on average 0.1% higher than those from (GAii), and the Maximum 319 Absolute Error values are 1.6% higher. 320

A limitation of the approach is that the Fit to Median Error measure will perform best at improving fit to the ground truth on datasets which violate the assumptions stated in section 1; the ship powering example is chosen to illustrate this as it provides a clearly heteroscedastic dataset with a cubic speed-power relationship. For applications where noise profiles are Gaussian, and there are no latent or interrelated input variables, the Fit to Median Error will

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not improve the fit to ground truth but will perform the same as conventional Minkowski-r metrics, either Mean Squared or Mean Absolute Error depending on the convexity of input-output relationships.

Interestingly, the approach producing the lowest Mean Absolute and Max-330 imum Absolute Errors does not model the ground truth the most accurately. 331 This creates a potential for negative societal impacts, as the standard perfor-332 mance metrics for regression neural networks do not provide a full picture of 333 performance or expected behaviour. Accurate input-otput relationships are essential for safe applications of machine learning in the real world, especially 335 when automated methods are used to replace experienced professionals. (GAii) 336 demonstrates the same accuracy of approach as those with standard network 337 regularisation, but with a better fit to the ground truth. This approach bypasses 338 the need to use, and therefore to optimise the parameters of the regularisation methods. If evolutionary computation is already being used to optimise network 340 parameters, then compute is saved by removing the network regularisation pa-341 rameters 11, 12 and dropout. (GAiii) completed 300 generations in 46hours 342 whereas (GAii) required 12 hours more computation to complete 300 generations.

#### 345 8. Conclusion

The error measures used in our current Machine Learning approaches can 346 provide an accurate point-wise estimate, without being able to approximate the input-output relationships in many real world datasets. New error measures are applied that match to the expected mean under less restrictive conditions. 349 Three different approaches are compared: one to minimise the Maximum Ab-350 solute Error of the networks, which includes standard regularization using 11, 351 12 and dropout; and two which do not use any network regularisation, one minimising the Mean Fit to Median and one to minimise the Maximum Absolute Error. The results show that all three approaches give similar Mean Absolute 354 Errors from networks on their Pareto fronts, from 2.9% for the approach with 355 regularisation to 3.1% for the approach minimising Maximum Absolute Error.

However, using a new measure, the Mean Fit to the Median, a considerably better approximation of the expected mean can be made, with a spread in pre-358 dicted input-output curves of 3% compared to a spread of 6% for the approach using regularisation and 10% when minimising the Maximum Absolute Error and where it is the only approach where the input-output curves don't cross. 361

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